



# Degradation and device physics modeling of SWCNT/CdTe thin film photovoltaics



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## ABSTRACT

We propose single walled carbon nanotubes as the n-type window partner of CdTe layer in a conventional CdS/CdTe thin film solar cells. The semiconductor nanotubes have superior optical and electrical properties i.e. controllable high band gap, being highly conductive and non-diffusive (not mobile). We modeled current–voltage characteristics of hybrid SWCNT/CdTe structure using Sah–Noyce–Shockley theory instead of Schottky barrier theory. The former theory is rather strong since it is based on carrier transport in the depletion region of a pn junction and considers the defect density within the depletion width. Also, a time dependent approach is used to simulate the degradation of device metrics under bias, illumination and temperature. It is discussed how a nanolayer can reduce the degradation rate of a thin film solar cell by surpassing grain boundaries and mobile ions migration towards junction.

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## 1. Introduction

Some research group proposed the application of Carbon Nanotubes (CNTs) in the solar cells because it would mean lighter panels, lower costs and easier to make products. They've been hampered, however, by the limited amount of power that such cells are able to generate high efficiencies. Excellent optical and electronic properties of CNTs such as direct band gap, high mobility, and efficient delivery of dissociated charge carriers to the electrode at high speed, high optical response and stability at higher temperatures make it an interesting material for the photovoltaic applications [1]. The physical structure of CNTs has two different electronic properties: semiconductor and metallic. Recently, we have considered the application of CNT as the buffer layer of chalcogenide thin film solar cells where CNT can increase the open circuit voltage of the device by reducing the recombination rate at the junction of p-type CIGS and n-type CdS [3]. However, so far the performance obtained from this hybrid device is quite low and the degradation/stability under different temperature and bias or illumination levels is to be investigated yet. The software package solves the coupled Poisson and continuity equations [4]. A few simulation analyses were performed using AMPS-1D and SCAPS for hybrid devices of Nanotube layers and their degradation rate was related to defect increment at the junction [5]. CNT plays the role of a heterojunction component for charge separation within the depletion region as CNT layer can be a high conductive partner for CdTe [6]. Along with our prior works on semiconductor quantum dot and thin film CdTe solar cells [7–10], in this paper we study on a hybrid heterostructure of CNT/CdTe. The reason why we choose SWCNT instead of multi-WCNTs is its lower lateral resistance. Then the lower conductivity of nanolayer

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increases the series resistance at the junction and the overall performance will reduce due to a lower fill factor. Note that the carriers have to transport via the nanotube and reach the respective electrodes. A theoretical model is presented based on the generation-recombination within the depletion width. Then a time dependent approach is used to model the device degradation rate. This theory was recently developed by our group for ultrathin film solar cells of CdS/CdTe materials [4]. AMPS stands for Analysis of Microelectronic and Photonic Structures. It was engineered to be a very general and versatile computer simulation tool for the analysis of device physics and device design. It is a one-dimensional (1-D) device physics program which is applicable to any 2-terminal device. It serves for diode, sensor, photo-diode, and photovoltaic device analysis. The time dependent approach was newly developed in AMPS-1D and SCAPS-1D simulators and is applied here as a rare numerical approach to study the device degradation as the available simulators to the PV community [11].

In 2007, NREL scientists used SWCNTs as back contact in the near-infrared transparent CdTe solar cells since SWCNT networks are hole-selective conductors and have a significantly greater transparency than TCOs [12]. They also suggested that the high transparency of SWCNTs could make them very useful in tandem thin-film solar cells. SWCNT networks can be incorporated into single-junction CdTe devices and in CdTe top cells for mechanically stacked thin-film tandem devices. SWCNT back contacted devices showed 12.4% efficiency by 40%–50% transmission rate for the wavelength range of 800–1500 nm. Nevertheless, it is not immediately clear why the SWCNT back contacted devices are less efficient. The lower performance comes from the reduced short-circuit current density and fill factor. On the other hand, an increased open circuit voltage is notable which can be associated with the number of factors, including the optical transmission, reflection, and absorption spectra of SWCNT networks. Results of the Ref. [12] encouraged the same researchers in NREL to incorporate the SWCNT in their tandem cells [13]. In a rather advanced study, they reported that SWCNTs produced at NREL by pulsed laser vaporization are sufficiently conductive to produce reasonable device efficiency (7.2%). They inserted ZnTe:Cu layer as the buffer too.

A review in literature reports on the fabrication of CdS/CdTe thin film solar cells using SWCNT as the back contact reveals performance and stability. A list of literature reports in Refs. [15–20] is presented in Table 1.

The difference between the structures indicated in Table 1 with the one presented in Fig. 1 is the CdS layer which has been omitted in schematic diagram of CdTe/SWCNT.

## 2. Theory

According to the Sah–Noyce–Shockley theory, the generation-recombination rate in the depletion layer at bias voltage  $V$  is given by,

$$U(x, V) = \frac{n(x, V)p(x, V) - n_1^2}{\tau_{po}[n(x, V) + n_1] + \tau_{no}[p(x, V) + p_1]}, \quad (1)$$

where  $n(x, V)$  and  $p(x, V)$  are the concentrations of free carriers in the conduction and valence bands,  $n_0$  and  $p_0$  are their equilibrium values, and  $\tau_{no}$  and  $\tau_{po}$  are the “effective” lifetimes of the electrons and holes in the space-charge region, respectively. The quantities  $n_1 = N_c \exp(-E_t/kT)$  and  $p_1 = N_v \exp(-E_t - E_g/kT)$  equal to the equilibrium concentrations of electrons and holes when the Fermi level, coincides with the recombination-center level  $N_c = 2(m_n kT/2\pi\hbar^2)^{3/2}$  and  $N_v = 2(m_p kT/2\pi\hbar^2)^{3/2}$  being the effective density of states in the conduction and valence bands,  $m_n$  and  $m_p$  being the effective mass of electrons and holes, respectively,  $E_t$  is the energy spacing between the recombination level and the conduction-band bottom. The recombination current under forward bias and the generation current under reverse bias are found by integrating  $U(x, V)$  over the entire space-charge region. Let us adapt the Sah–Noyce–Shockley model, developed for p–n junction, to the Schottky diode based on n-type semiconductor where here the n-type is SWCNT with a band alignment similar to CdS layer in a regular CdS/CdTe device. In this case, the width of the space charge region is given by

$$W = \sqrt{\frac{2\epsilon\epsilon_0(\phi_0 - qV)}{e^2(N_d - N_a)}}, \quad (2)$$

**Table 1**

An overview on the performance and stability of thin film PVs hybrid with a nanolayer.

Device structure	$J_{sc}$ (mA/cm <sup>2</sup> )	$V_{oc}$ (V)	FF (%)	$\eta$ (%)	Ref.
1. glass/MO/CIGS/CdS/SWCNT	35.34	0.693	79.4	19.5	[15]
2. glass/TCO/ZTO/CdS/CdTe/CuTe/SWCNT	22.25	0.818	68.1	12.4	[16]
3. glass/TCO/CdS/CdTe/ZnTe:Cu/SWCNT	21.30	0.800	42.2	7.2	[17]
8. glass/TCO/CdS/CdTe/Au-SWCNT	21.15	0.773	76.2	11	[18]
9. glass/TCO/CdS/CdTe/SWCNT	19.70	0.795	70.4	11	[19]
10. glass/TCO/CdS/CdTe/C-SWCNT	25.00	0.829	68	14.1	[20]

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